

Exercise 4

1. Compare the following phenol manufacturing processes using the appropriate green chemistry metrics and using the green chemistry principles: benzene sulfonation, benzene chlorination, Hock process.
2. Discuss the advantages of the following alternative processes in terms of greenness: Solutia and ExxonMobil processes

Chemical	MW	Sulfonation		Chlorination		Hock		Solutia		ExxonMobil	
		mol	g	mol	g	mol	g	mol	g	mol	g
Benzene	78.1	-1	-78.1	-1	-78.1	-1	-78.1	-1	-78.1	-2	-156.2
Phenol	94	1	94	1	94	1	94	1	94	1	94
NaHSO ₃	104	2	208.2								
Na ₂ SO ₃	126	-1	-126								
Na ₂ SO ₃	126	1	126								
SO ₂	64.1	-1	-64.1								
NaOH	40	-2	-80	-1	-40						
H ₂ O	18	2	36								
Cl ₂	70.9			-1	-70.9						
HCl	36.5			1	36.5						
NaCl	58.4			1	58.4						
Propene	42.1					-1	-42.1				
Oxygen	32					-1	-32			-1	-32
Acetone	58.1					1	58.1				
N ₂ O	44							-1	-44		
N ₂	28							1	28		
Hydrogen	2									-2	-4
H ₂ SO ₄	98.1	-1	-98.1								
Cyclohexanone	98.1									1	98.1
AE			21.1%		49.7%		61.8%		77.0%		48.9%
AE with valorizable by-product							100%		100%		100%
Ideal E-factor (=1/AE-1)			3.9		1.0		0.6		0.3		1.0
Ideal E-factor (with co-product valorization)			3.9		1.0		0.0		0.0		0.0
Co-products		NHSO ₃ , Na ₂ SO ₃		HCl, NaCl		acetone		N ₂ (valorizable)		cyclohexanone	
By-products				para-phenyl-phenol, di-phenylether		acetophenone, alpha methylstyrene		<5%		<3%	
Catalytic?		No		No		Yes		Yes		Yes	
Toxic raw materials other than benzene?		Yes		Yes		No		No		No	

Main green chemistry principles addressed by Hock, Solutia and ExxonMobil processes

- 1: Prevent waste
- 2: Atom economy
- 3: Less hazardous synthesis

8: Reduce derivatives

9: Catalysis (vs. stoichiometric)